

Departmental Seminar - Chemistry Visiting Student

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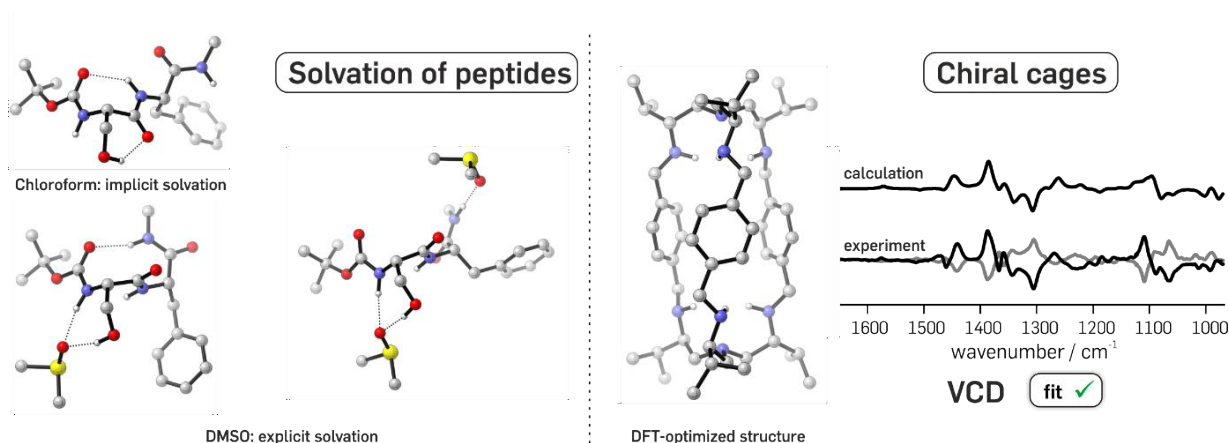
(Dept. of Chemistry Supervisor: Dr. Travis Fridgen)

Thursday, March 14 at 1:00 p.m. (Rm: CSF-1302)

Title:

Vibrational Circular Dichroism (VCD) Spectroscopy: A Tool to Elucidate Solution-Phase Structures of Chiral Molecules

Abstract:



Vibrational Circular Dichroism (VCD) spectroscopy is the chiral version of IR spectroscopy. The difference in the absorbance of left- and right-circularly polarized light is measured. Unlike electronic CD spectroscopy, no special chromophore groups are needed for this technique. As molecular vibrations are probed, each bonded atom becomes a chromophore. Thus, every chiral molecule can be studied with VCD spectroscopy.

The method can be used to determine the absolute configuration of chiral molecules. Moreover, in contrast to simple IR spectroscopy, VCD spectroscopy is very sensitive to conformational changes making it an ideal tool to investigate preferred conformations in solution. This technique relies heavily on quantum-mechanical calculations. The geometries of the analytes are first optimized with DFT-based methods and then the harmonic frequencies are calculated. The experimental spectra are compared with the calculated spectra in a subsequent step.

In our group, we have investigated the solution-phase structures of serine-based peptides in different solvents. The population of conformer families depend on the hydrogen-bonding capabilities of the solvent. In general, intramolecular hydrogen bonds remain in chloroform and are partly broken in the hydrogen-bond acceptor DMSO. More complex mixed solvation states are present.^[1]

In another project chiral cages based on chiral tripodal tris-(2-aminoethyl)-amine (TREN) molecules have been synthesized. Those molecules are capable of encapsulating metal cations and small organic

anions. The solution phase structure of these cages has been investigated by VCD spectroscopy.^[2]

References:

- [1] C. Müller, C. Merten, *Physical chemistry chemical physics : PCCP* **2023**, 25, 19462.
- [2] C. Müller, K. Scholten, E. Engelage, C. Merten, *Chemistry – A European Journal* **2023**, 29, e202302126.